

alpha-Humulene
6753-98-6 | DTXSID30858793

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.09e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.20e-01

Confidence level: 8.07e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3-Phenylprop-2-enal</div> <div>Measured: 1.28e-03</div> <div>Predicted: 8.01e-02</div>	<div>Image not found</div> <div>Benzene, hexyl-</div> <div>Measured: 5.71e-03</div> <div>Predicted: 7.69e-02</div>	<div>Image not found</div> <div>R-(-)-Carvone</div> <div>Measured: 2.42e-04</div> <div>Predicted: 1.33e-01</div>
<div>Image not found</div> <div>Octabromodibenzo-p-dioxin</div> <div>Measured: 1.13e-02</div> <div>Predicted: 5.47e-13</div>	<div>Image not found</div> <div>Simazine</div> <div>Measured: 5.11e-05</div> <div>Predicted: 1.09e-07</div>	